Static dielectric function with exact exchange contribution in the electron liquid

Zhixin Qian

Department of Physics, Peking University, Beijing 100871, China

(Dated: August 4, 2015)

The exchange contribution, $\Pi_1(\mathbf{k},0)$, to the static dielectric function in the electron liquid is evaluated exactly. Expression for it is derived analytically in terms of one quadrature. The expression, as presented in Eq. (3) in the Introduction, turns out to be very simple. A fully explicit expression (with no more integral in it) for $\Pi_1(\mathbf{k},0)$ is further developed in terms of series. Equation (3) is proved to be equal to the expression obtained before under some mathematical assumption by Engel and Vosko, thus in the meanwhile putting the latter on a rigorous basis. The expansions of $\Pi_1(\mathbf{k},0)$ at the wavectors of $k=0$, $k=2k_F$, and at limiting large k are derived. The results all verify those obtained by Engel and Vosko.

PACS numbers: 71.15.Mb, 71.10.-w, 71.45.Gm

I. INTRODUCTION WITH CONCLUDING REMARKS

The dielectric function in the homogeneous electron liquid is determined by [1, 2]

$$\epsilon(\mathbf{k},\omega) = 1 - v(k)\Pi(\mathbf{k},\omega); \tag{1}$$

$\Pi(\mathbf{k},\omega)$ is the proper (irreducible) linear response function. [$v(k)$ is the Fourier transform of the Coulomb potential.] Many electronic properties in solids and liquids can be described from the dielectric function. Rapid developments in the techniques of inelastic x-ray scattering and electron energy-loss spectroscopies in recent years [3–7] now enable us to measure these dielectric function related properties with unprecedented accuracy.

Theoretically, Lindhard [8] obtained, about six decades ago, the explicit expression for $\Pi_0(\mathbf{k},\omega)$, the zeroth-order of $\Pi(\mathbf{k},\omega)$ in terms of Coulomb interaction, in the homogeneous electron gas; wherefore it is also known as Lindhard function. Keeping $\Pi_0(\mathbf{k},\omega)$ only in Eq. (1) yields the random phase approximation (RPA) [1, 9] for $\epsilon(\mathbf{k},\omega)$. An enormous amount of effort had been devoted to the study of the correction beyond RPA since the pioneering proposals made by Hubbard [10] (and DuBois [11]). The correction beyond RPA is fully due to the exchange-correlation effects, which is also termed, according to Hubbard, as local field correction $G(\mathbf{k},\omega)$:

$$G(\mathbf{k},\omega) = v(k)^{-1}\left[\frac{1}{\Pi(\mathbf{k},\omega)} - \frac{1}{\Pi_0(\mathbf{k},\omega)}\right]. \tag{2}$$

Needless to say, the lowest order correction, $\Pi_1(\mathbf{k},\omega)$, to the Lindhard function, which is traditionally also known as the exchange contribution to $\Pi(\mathbf{k},\omega)$, had been of major research interest [12–22]. In some of the researches, not strictly $\Pi_1(\mathbf{k},\omega)$ but variants of it were studied as well. Higher order contributions beyond $\Pi_0(\mathbf{k},\omega)+\Pi_1(\mathbf{k},\omega)$ had also been studied, for instance, in Refs. [12, 19]. About two and a half decades ago, Engel and Vosko [23] obtained an analytical expression [Eq. (29) in Ref. [23]] for $\Pi_1(\mathbf{k},0)$ in terms of one quadrature. That was definite progress, and one must be aware that the original form for $\Pi_1(\mathbf{k},0)$ is in six-fold integral [see Eq. (5) in the next section]. Indeed, most of the work we mentioned above relied on numerical procedures in one way or another. Unfortunately the derivation by Engel and Vosko can not be fully regarded as rigorous in that it critically relies on some mathematical assumption. But convergence to the numerical results for $\Pi_1(\mathbf{k},0)$ and many right analytical features all strongly suggest the correctness of their expression. Very encouragingly in this connection, Glasser [24] confirmed Eq. (29) of Ref. [23] with the aid of analytical computer programs. Several of the leading terms in the small wavevector expansion of $\Pi_1(\mathbf{k},0)$ obtained from it were also confirmed later analytically by Svendsen and von Barth [25].

In this paper we report an exact evaluation of $\Pi_1(\mathbf{k},0)$. The main result of the present work is the following expression for $\Pi_1(\mathbf{k},0)$,

$$\Pi_1(\mathbf{k},0) = \frac{m^2e^2}{2\pi^3k^2}\left[b\ln^2\left|\frac{b}{a}\right|\left(\frac{1}{3}a\ln\left|\frac{b}{a}\right| + b\right) + \int_{a^2}^{b^2} dx\frac{1}{x-a^2}\ln\left|\frac{x}{a^2}\right|\left(\frac{1}{2}ab\ln\left|\frac{x}{b^2}\right| - k\right)\right], \tag{3}$$

with $a = 1-k/2$, $b = 1+k/2$, and k in units of k_F. The result for $\Pi_1(\mathbf{k},0)$ can be claimed to be surprisingly simple. Equation (3) is proved to be equal to the one given by Engel and Vosko [23] mentioned above; but in

the present work it is derived rigorously. The expansions of it at $k = 0$, $k = 2$, and at limiting large k are also derived; they fully confirm the corresponding ones obtained in Ref. [23].

The remaining integral in Eq. (3) is a straightforward numerical task. But we have an interesting alternative which is to further carry out *analytically* the remaining integral in terms of series. In this way, a fully explicit expression for $\Pi_1(\mathbf{k}, 0)$ is developed, which is shown in Eq. (93) in Sec. V, with the quantity I(k) being related to $\Pi_1(\mathbf{k}, 0)$ as in Eq. (6), and $\zeta(3)$ being Riemann's zeta function. This series representation should be suitable for both of numerical and analytical applications.

The details of our derivation are given in Sections II-IV; supporting materials are relegated to Appendices A and B. The final result is given in Sec. V in which the above-mentioned series representation is also developed. The proof of the equivalence of our result and Eq. (29) in Ref. [23] is given in Sec. VI. The expansions of $\Pi_1(\mathbf{k}, 0)$ in limiting cases are derived in Sec. VII.

II. REDUCTION OF $\Pi_1(\mathbf{k}, 0)$ TO TWO-DIMENSIONAL INTEGRAL

Explicit expression for $\Pi_1(\mathbf{k}, \omega)$ can be obtained with the diagrammatic techniques [11] (see also Refs. [12, 19]):

$$\Pi_1(\mathbf{k},\omega) = 2\int \frac{d\mathbf{p}}{(2\pi)^3}\frac{d\mathbf{p}'}{(2\pi)^3} v(\mathbf{p}-\mathbf{p}')\frac{(n_{\mathbf{p}}-n_{\mathbf{p}+\mathbf{k}})(n_{\mathbf{p}'}-n_{\mathbf{p}'+\mathbf{k}})}{\omega+\omega_{\mathbf{p}}-\omega_{\mathbf{p}+\mathbf{k}}+i0^+}\left[\frac{1}{\omega+\omega_{\mathbf{p}}-\omega_{\mathbf{p}+\mathbf{k}}+i0^+}-\frac{1}{\omega+\omega_{\mathbf{p}'}-\omega_{\mathbf{p}'+\mathbf{k}}+i0^+}\right], \tag{4}$$

where $\omega_{\mathbf{p}} = p^2/2m$ and $n_{\mathbf{p}}$ is the Fermi-Dirac distribution function. (We put $\hbar = 1$ in this paper.) At $\omega = 0$, one gets

$$\Pi_1(\mathbf{k},0) = -8\pi m^2 e^2 \int \frac{d\mathbf{p}}{(2\pi)^3}\int \frac{d\mathbf{p}'}{(2\pi)^3} n_{\mathbf{p}-\mathbf{k}/2} n_{\mathbf{p}'-\mathbf{k}/2}\left[\left(\frac{1}{\mathbf{p}\cdot\mathbf{k}}+\frac{1}{\mathbf{p}'\cdot\mathbf{k}}\right)^2\frac{1}{|\mathbf{p}+\mathbf{p}'|^2}-\left(\frac{1}{\mathbf{p}\cdot\mathbf{k}}-\frac{1}{\mathbf{p}'\cdot\mathbf{k}}\right)^2\frac{1}{|\mathbf{p}-\mathbf{p}'|^2}\right]. \tag{5}$$

The $\Pi_1(\mathbf{k}, 0)$ in Eq. (5) is equal to the corresponding one defined in Ref. [23]. We also define $I(k)$ as

$$I(k) = \frac{\pi^3}{m^2 e^2}\Pi_1(\mathbf{k}, 0). \tag{6}$$

We note that $\Pi_1(\mathbf{k}, 0)$ depends only on the magnitude k in a uniform system. $I(k)$ so defined has the well-known property of $I(k = 0) = -1$ (see Sec. VII).

We shall perform our calculation in the cylindrical coordinates. The advantage of the cylindrical coordinates in calculating $\Pi_1(\mathbf{k}, \omega)$ had been appreciated before [18, 21, 23, 24, 26]. The integrals over the azimuthal angular variables of $\mathbf{p}$ and $\mathbf{p}'$ can be readily carried out. After that one obtains

$$I(k) = -\frac{1}{8k^2}\int_{-a}\int^{b} dz dz' \frac{1}{z^2 z'^2}[\alpha^2 L(\alpha^2) - \beta^2 L(\beta^2)], \tag{7}$$

where $\alpha = z + z'$, $\beta = z - z'$. The same notations as those in Ref. [24] are adopted. The function L in Eq. (7) is defined as

$$L(u) = \int_0^{\lambda} dx \int_0^{\lambda'} dx' \frac{1}{\sqrt{(x-x')^2 + 2(x+x')u + u^2}}, \tag{8}$$

where $\lambda = (a + z)(b - z)$ and $\lambda' = (a + z')(b - z')$. The two-dimensional integral on the right hand side of Eq. (8) can be further carried through. The resulting expression for $L(u)$ is

$$\begin{aligned} L(u) &= \frac{1}{2}[L_1(u) - (\lambda+\lambda')(1 + 2\ln|2u|) - u] \\ &+ \lambda \ln|L_1(u) + \lambda' - \lambda + u| \\ &+ \lambda' \ln|L_1(u) + \lambda - \lambda' + u|, \end{aligned} \tag{9}$$

where

$$\begin{aligned} L_1(u) &= \sqrt{(\lambda' - \lambda + u)^2 + 4\lambda u} \\ &= \sqrt{u^2 + (\lambda - \lambda')^2 + 2(\lambda + \lambda')u}. \end{aligned} \tag{10}$$

Substituting Eq. (9) into Eq. (7), one obtains

$$I(k) = -\frac{1}{16k^2}\sum_{i=0}^{3} J_i, \tag{11}$$

where

$$J_0 = -4\int_{-a}\int^{b} dz dz' \frac{1}{zz'}[(\lambda+\lambda')(2\ln 2 + 1) + \alpha^2 + \beta^2]; \tag{12}$$

$$J_1 = \int_{-a}\int^{b} dz dz' \frac{1}{z^2 z'^2}[\alpha^2 L_1(\alpha^2) - \beta^2 L_1(\beta^2)]; \tag{13}$$

$$J_2 = 2\int_{-a}\int^{b} dzdz'\frac{1}{z^2 z'^2} \quad \{ \quad \lambda[\alpha^2 \ln|L_1(\alpha^2)+\lambda'-\lambda+\alpha^2| - \beta^2 \ln|L_1(\beta^2)+\lambda'-\lambda+\beta^2|] \\ + \quad \lambda'[\alpha^2 \ln|L_1(\alpha^2)+\lambda-\lambda'+\alpha^2| - \beta^2 \ln|L_1(\beta^2)+\lambda-\lambda'+\beta^2|]\}, \tag{14}$$

or, by the use of the fact that both of $L_1(\alpha^2)$ and $L_1(\beta^2)$ remain unchanged [in virtue of the second identity in Eq. (10)] upon exchanging z and z',

$$J_2 = 4\int_{-a}\int^{b} dzdz'\frac{1}{z^2 z'^2}\lambda[\alpha^2 \ln|L_1(\alpha^2)+\lambda'-\lambda+\alpha^2| - \beta^2 \ln|L_1(\beta^2)+\lambda'-\lambda+\beta^2|]; \tag{15}$$

and

$$J_3 = 4\int_{-a}\int^{b} dzdz'\frac{1}{z^2 z'^2}\lambda[\beta^2 \ln|\beta^2| - \alpha^2 \ln|\alpha^2|]. \tag{16}$$

J_0 can be evaluated to be

$$J_0 = -8\ln|b/a|[ab(1+2\ln 2)\ln|b/a| + k(3+\ln 2)], \tag{17}$$

and accordingly

$$I(k) = -\frac{1}{16k^2}\{ \quad - \quad 8\ln|b/a|[ab(1+2\ln 2)\ln|b/a| \\ + \quad k(3+2\ln 2)] + \sum_{i=1}^{3} J_i\}. \tag{18}$$

The J_1, J_2, and J_3 are the same as the ones defined in Ref. [24]. The expression for J_1 here appears to be different to that in Ref. [24] but is actually equal. There is an extra term of the following form,

$$\int_{-a} dz \int^{b} dz' \frac{1}{z^2 z'^2}(\lambda'-\lambda)[L_1(\alpha^2) - L_1(\beta^2)], \tag{19}$$

in the expression for J_1 in Eq. (10) of Ref. [24], but this extra term can be shown to be equal to zero. (We note that in our foregoing derivation this term did not arise at all.) In fact, the factor of $\lambda - \lambda'$ changes sign but that of $L_1(\alpha^2) - L_1(\beta^2)$ [actually each of $L_1(\alpha^2)$ and $L_1(\beta^2)$] remains unchanged upon exchanging z and z' as mentioned above. In consequence,

$$\int_{-a} dz \int^{b} dz' \frac{1}{z^2 z'^2}(\lambda'-\lambda)[L_1(\alpha^2) - L_1(\beta^2)] = 0. \tag{20}$$

Understandably, this term with null contribution might however cost a huge amount of labor in any further numerical or analytical calculations if not appreciated.

The expression for $I(k)$ has as a consequence been successfuly reduced in terms of two-dimensional integral. Similar type of reduction had been accomplished or applied in Refs. [18, 21–24, 26]. (Brosens et al. [18] in fact considered both of the static and dynamic cases.) A different approach was adopted by Holas et al. [19] who essentially first calculated the imaginary part of $\Pi_1(\mathbf{k}, \omega)$, and then the real part of it [with the static $\Pi_1(\mathbf{k}, 0)$ as its special case] via the dispersion relation, which virtually also amounts to a two-dimensional integral over all. The remaining two-dimensional integral was then calculated numerically in Refs. [18, 19, 21, 22, 26]; analytically with the aid of some ingenious method and mathematical assumption in Ref. [23]; and analytically but with computer programs in Ref. [24]. We need point out that there exists discrepance between our Eq. (18) and the corresponding expression in Ref. [24] [the one shown in the middle of the paragraph above Eq. (10) in Ref. [24]].

III. EVALUATION FOR J_1

It turns out that the integral in Eq. (13) for J_1 can be *fully* carried through. We are about to achieve this step by step. Indeed, either the integral over z or z' can be carried out first. But before doing that it is worth pointing out a somewhat hidden but useful truth. $L_1(\beta^2)$ can actually be, by direct substitution in Eq. (10), simplified to the following form:

$$L_1(\beta^2) = 2|\beta|. \tag{21}$$

Accordingly J_1, with some further algebra, can be written as

$$J_1 = 4\int_{-a}^{b} dz\frac{1}{z^2}\int_{-a}^{b} dz'\frac{1}{z'}[\alpha\sqrt{R(z,z')} + \beta|\beta|], \tag{22}$$

where

$$R(z,z') = C_0(z)z'^2 + B_0(z)z' + A_0(z), \tag{23}$$

with

$$A_0(z) = z^2,\ B_0(z) = (2+2kz-k^2)z,\ C_0(z) = 1+2kz. \tag{24}$$

For brevity, $A_0(z)$, $B_0(z)$, and $C_0(z)$ will be denoted, respectively, as A_0, B_0, and C_0 instead, i.e., with the argument z suppressed. We next define

$$\bar{J}_1^A(z) = \int_{-a}^{b} dz'\frac{1}{z'}\alpha\sqrt{R(z,z')}, \tag{25}$$

and

$$\bar{J}_1^B(z) = \int_{-a}^{b} dz' \frac{1}{z'} \beta|\beta|, \tag{26}$$

so that we can write J_1 as

$$J_1 = 4\int_{-a}^{b} dz \frac{1}{z^2}[\bar{J}_1^A(z) + \bar{J}_1^B(z)]. \tag{27}$$

The integration over z' on the right hand side of Eq. (26) for $\bar{J}_1^B(z)$ presents no analytical difficulty. It is straightforward and the resulting expression is,

$$\bar{J}_1^B(z) = 2kz - 1 - k^2/4 - z^2(3 - 2\ln|z| + \ln|ab|). \tag{28}$$

On the other hand, the integration in $\bar{J}_1^A(z)$ is more subtle, but becomes also routine [27] if we rewrite it as

$$\bar{J}_1^A(z) = z\int_{-a}^{b} dz' \frac{1}{z'}\sqrt{R(z,z')} + \int_{-a}^{b} dz' \sqrt{R(z,z')}. \tag{29}$$

Each of the integrations in Eq. (29) can be carried through, and the result for $\bar{J}_1^A(z)$ is

$$\begin{aligned}\bar{J}_1^A(z) &= 1 + \frac{1}{4}k^2 + \frac{5}{2}kz + 2z^2 + \frac{B_0}{4C_0}(2z+k)\\ &- z|z|\ln\left|\frac{a\psi_1(z)}{b\psi_2(z)}\right|\\ &+ \frac{1}{2}\left(zB_0 + A_0 - \frac{B_0^2}{4C_0}\right)\frac{1}{\sqrt{C_0}}\ln\left|\frac{\psi_3(z)}{\psi_4(z)}\right|,\end{aligned} \tag{30}$$

where

$$\psi_1(z) = 2A_0 + B_0 b + 2\sqrt{A_0 R(z,b)}, \tag{31}$$

$$\psi_2(z) = 2A_0 - B_0 a + 2\sqrt{A_0 R(z,-a)}, \tag{32}$$

$$\psi_3(z) = 2\sqrt{C_0 R(z,b)} + 2C_0 b + B_0, \tag{33}$$

and

$$\psi_4(z) = 2\sqrt{C_0 R(z,-a)} - 2C_0 a + B_0. \tag{34}$$

$R(z,b)$ and $R(z,-a)$ can be written explicitly in the following forms,

$$R(z,b) = [(1+k)z + b]^2;\;\; R(z,-a) = [(k-1)z + a]^2. \tag{35}$$

Equation (27), together with the explicit expressions (28) for $\bar{J}_1^B(z)$ and (30) for $\bar{J}_1^A(z)$, indicates that we have already reduced J_1 in terms of one quadrature. Further analytical refinement turns out to be practicable, but only after one finds a way to simplify the somewhat unwieldy quantities $\psi_1(z)/\psi_2(z)$ and $\psi_3(z)/\psi_4(z)$. Indeed, we find the following simple expressions for them:

$$\frac{\psi_1(z)}{\psi_2(z)} = \left(\frac{2b}{k}\right)^2\theta(z) + \left(\frac{k}{2a}\right)^2\theta(-z), \tag{36}$$

where $\theta(z) = 1$ for $z > 0$ and $\theta(z) = 0$ for $z < 0$; and

$$\frac{\psi_3(z)}{\psi_4(z)} = \left(\frac{\sqrt{C_0}+1}{\sqrt{C_0}-1}\right)^2. \tag{37}$$

The simplifications play a critical role in our further reducing J_1 to a fully explicit form [Eq. (42) below]. The verification for Eq. (36) and Eq. (37) is given in Appendix A. We here substitute them into Eq. (30) to obtain

$$\begin{aligned}\bar{J}_1^A(z) &= 1 + \frac{1}{4}k^2 + \frac{5}{2}kz + \left(2 - \ln\left|1 - \frac{4}{k^2}\right|\right)z^2\\ &+ \frac{B_0}{4C_0}(2z+k)\\ &+ \frac{1}{4C_0^{3/2}}z^2[8 - k^4 + 4kz(6-k^2) + 12k^2z^2]Y(z),\end{aligned} \tag{38}$$

where we have adopted the following notation,

$$Y(z) = \ln\left|\frac{\sqrt{C_0}+1}{\sqrt{C_0}-1}\right|. \tag{39}$$

We then substitute Eqs. (28) and (38) into Eq. (27) and, with some further routine calculation, obtain

$$\begin{aligned}J_1 = &- 20 + 16\ln k + \frac{2}{k}(k^2-1)^2\ln\left|\frac{k+1}{k-1}\right|\\ &- (k^3 - 24k + 8)\ln|2b|\\ &+ (k^3 - 24k - 8)\ln|2a|\\ &+ \frac{1}{k}[3\eta_1 + 2(3-k^2)\eta_{-1} - (k^2-1)^2\eta_{-3}],\end{aligned} \tag{40}$$

where

$$\eta_n = k\int_{-a}^{b} dz C_0^{n/2} Y(z). \tag{41}$$

The explicit expressions for η_1, η_{-1}, and η_{-3} are given in Eq. (B2), Eq. (B3), and Eq. (B4), respectively. By substituting Eqs. (B2), (B3), (B4) into Eq. (40), we obtain our final result for J_1:

$$J_1 = -16 + 4(5k + 4/k)\ln|b/a|. \tag{42}$$

The result is surprisingly elegant.

IV. EVALUATION FOR $J_2 + J_3$

Among the three expressions as shown in (13), (15), and (16), the expression in (13) for J_1 is likely the one the most amenable to analytical computations. This is in fact also the cause that it can be fully reduced to the explicit expression of (42). On the other hand, due to the logarithm forms in them, Eq. (15) and Eq. (16) are much more difficult. Further reduction of J_2 and

J_3, at least that of J_2 , to one quadrature, had been believed beyond barehanded effort [24]. We find indeed that careless choices of procedures might easily make the task intractable. It is critical to search for optimal ones.

Instead of evaluating J_2 and J_3 separately, we choose to combine them together and deal with them at one stroke. We write $J_{23}= J_2+J_3$, and accordingly have

$$J_{23} = 4\int_{-a}\int^{b} dzdz'\frac{\lambda}{z^2z'^2}\left\{\alpha^2\ln|[L_1(\alpha^2)+\lambda'-\lambda+\alpha^2]/\alpha^2| - \beta^2\ln|[a-b+2z+2\beta/|\beta|]/\beta|\right\}. \tag{43}$$

We have also made the use of Eq. (21) in obtaining the above equation. We next perform some manipulation on Eq. (43) to bring it into the following form:

$$J_{23} = 16\int_{-a}^{b} dz\frac{1}{z}\lambda\ln|4\lambda|\int_{-a}^{b} dz'\frac{1}{z'} - 4N, \tag{44}$$

where

$$N = \int_{-a}\int^{b} dzdz'\frac{\lambda}{z^2z'^2}[\alpha^2\ln|\alpha^2+\lambda'-\lambda-2\sqrt{R(z,z')}| - \beta^2\ln|\beta(a-b+2z-2\beta/|\beta|)|]. \tag{45}$$

The first term on the right hand side of Eq. (44) has virtually been reduced to a one-dimensional integral for the integration $\int_{-a}^{b} dz' 1/z'$ is trivial. Hence we need concern ourselves only with the term of $-4N$. For this purpose, we first rewrite N as the following:

$$N = \int_{-a}^{b} dz\frac{\lambda}{z^2}[\bar{N}_1(z) - \bar{N}_2(z)], \tag{46}$$

where

$$\bar{N}_1(z) = \int_{-a}^{b} dz'\frac{\alpha^2}{z'^2}\ln|\alpha^2+\lambda'-\lambda-2\sqrt{R(z,z')}|, \tag{47}$$

and

$$\bar{N}_2(z) = \int_{-a}^{z} dz'\frac{\beta^2}{z'^2}\ln|2\beta(z-b)| + \int_{z}^{b} dz'\frac{\beta^2}{z'^2}\ln|2\beta(z+a)|. \tag{48}$$

In the preceding expression for $\bar{N}_2$, the integral over z' has been purposely separated into two regimes of $-a \le z' < z$ and $z \le z' \le b$. This is intended to take care of the subtle singular behavior of the logarithm factor $\ln|\beta(a-b+2z-2\beta/|\beta|)|$ in Eq. (45). After performing partial integration on each of the integrals on the right hand sides of Eq. (47) and Eq. (48), one obtains

$$\begin{aligned}\bar{N}_1(z) = {}& 2\left(1-\frac{z^2}{ab}+z\ln\left|\frac{b}{a}\right|\right)\ln|2\lambda| \\ &+ \int_{-a}^{b} dz'\left(z'-\frac{z^2}{z'}+2z\ln|z'|\right) \\ &\times\frac{1}{\alpha}\left(\frac{kz}{\sqrt{R(z,z')}}-1\right),\end{aligned} \tag{49}$$

and

$$\begin{aligned}\bar{N}_2(z) = {}& 2\left(1-\frac{z^2}{ab}-z\ln\left|\frac{b}{a}\right|\right)\ln|2\lambda| + 2zW_1(z)\ln|z| \\ &+ \int_{-a}^{b} dz'\left(z'-\frac{z^2}{z'}-2z\ln|z'|\right)\frac{1}{\beta}.\end{aligned} \tag{50}$$

Here we have introduced the following notation,

$$W_1(z) = \ln\left|\frac{z+a}{z-b}\right|. \tag{51}$$

Equation (46), together with Eqs. (49) and (50), is then substituted into Eq. (44) to get

$$\begin{aligned}J_{23} = {}& 8(2\ln 2-1)(ab\ln|b/a|+k)\ln|b/a| \\ &+4(-k\Phi_1+2\Phi_2-2k\Phi_3+2\Phi_4),\end{aligned} \tag{52}$$

where

$$\Phi_1 = -\int_{-a}^{b} dz\frac{\lambda}{z}\int_{-a}^{b} dz'\frac{\beta}{z'}\frac{1}{\sqrt{R(z,z')}}, \tag{53}$$

$$\Phi_2 = -2\int_{-a}^{b} dz\frac{\lambda}{z}\int_{-a}^{b} dz'\frac{z'}{\alpha\beta}\ln|z'|, \tag{54}$$

$$\Phi_3 = \int_{-a}^{b} dz\lambda\int_{-a}^{b} dz'\frac{1}{\alpha\sqrt{R(z,z')}}\ln|z'|, \tag{55}$$

and

$$\Phi_4 = \int_{-a}^{b} dz\frac{\lambda}{z}W_1(z)\ln|z|. \tag{56}$$

Φ_4 is clearly not our concern temporarily, since it is already in terms of one-dimensional integral. Fortunately it turns out that the two-dimensional integral in Φ_1 can be fully carried through. We first attack it. To this end, we write

$$\Phi_1 = \int_{-a}^{b} dz \frac{\lambda}{z} \bar{\Phi}_1(z), \tag{57}$$

where

$$\bar{\Phi}_1(z) = \int_{-a}^{b} dz' \frac{1}{\sqrt{R(z,z')}} - z \int_{-a}^{b} dz' \frac{1}{z'\sqrt{R(z,z')}}. \tag{58}$$

Each of the integrals over z' in Eq. (58) is routine. After carrying out them, we obtain the following result for $\bar{\Phi}_1(z)$,

$$\bar{\Phi}_1(z) = \frac{z}{\sqrt{A_0}} \ln\left|\frac{a\psi_1(z)}{b\psi_2(z)}\right| + \frac{1}{\sqrt{C_0}} \ln\left|\frac{\psi_3(z)}{\psi_4(z)}\right|, \tag{59}$$

or, with the aid of Eqs. (36) and (37),

$$\bar{\Phi}_1(z) = \frac{2}{\sqrt{C_0}} Y(z) + \ln\left|\frac{4ab}{k^2}\right|. \tag{60}$$

Substitution of Eq. (60) into Eq. (57), followed by further algebra, yields

$$\Phi_1 = k(\ln|4ab| - 2\ln k) - \frac{1}{k^2}\eta_1 + \frac{1}{k^2}(1+2k^2)\eta_{-1}. \tag{61}$$

The use of Eqs. (B2) and (B3) in the above equation then yields

$$\begin{aligned}\Phi_1 = \quad & \frac{1}{3k^2}[(8k^3+9k^2+4)\ln b + (8k^3-9k^2-4)\ln|a| \\ & -4k + 16k^3 \ln|2/k|].\end{aligned} \tag{62}$$

This is another elegant result indeed.

Φ_2 in Eq. (54) and Φ_3 in Eq. (55) are our next concern. Clearly one can do nothing further directly with regard to integral over z' in those expressions, due to the simultaneous appearance of the factor $\ln|z'|$ and nontrivial denominator in each of the integrands. Our trick is to reverse the order of integrations over z and over z'. This means to perform the integration over z first instead of that over z'. This consideration yields the following form for Φ_2,

$$\Phi_2 = 2\int_{-a}^{b} dz z \ln|z| \int_{-a}^{b} dz' \frac{\lambda'}{z'} \frac{1}{\alpha\beta}. \tag{63}$$

Notice that we have exchanged the symbols of z and z' to obtain the preceding equation. The integration over z' can now be readily carried out. After that one obtains

$$\begin{aligned}\Phi_2 = \int_{-a}^{b} dz \frac{1}{z} \ln|z| \quad & [2ab\ln|b/a| + \lambda W_1(z) \\ & -(z^2+kz-ab)W_2(z)],\end{aligned} \tag{64}$$

where we have introduced the notation

$$W_2(z) = \ln\left|\frac{z-a}{z+b}\right|. \tag{65}$$

This temporarily finishes our job for Φ_2, for it is already in terms of one quadrature.

Next we consider Φ_3 of Eq. (55) in the same fashion. First notice the property

$$R(z,z') = R(z',z), \tag{66}$$

which enables us to rewrite Φ_3 as

$$\Phi_3 = \int_{-a}^{b} dz \bar{\Phi}_3(z) \ln|z|, \tag{67}$$

where

$$\bar{\Phi}_3(z) = \int_{-a}^{b} dz' \frac{\lambda'}{\alpha\sqrt{R(z,z')}}. \tag{68}$$

Explicitly,

$$\begin{aligned}\bar{\Phi}_3(z) \;=\; & (b+z)(a-z)\int_{-a}^{b} dz' \frac{1}{\alpha\sqrt{R(z,z')}} \\ + \; & (k+z)\int_{-a}^{b} dz' \frac{1}{\sqrt{R(z,z')}} - \int_{-a}^{b} dz' \frac{z'}{\sqrt{R(z,z')}}.\end{aligned} \tag{69}$$

Each of the integrals in Eq. (69) is routine. They can be carried through and the result is

$$\begin{aligned}\bar{\Phi}_3(z) = \quad & \frac{4-(k+2z)^2}{4k|z|}\left[\ln\left|\frac{\phi_1(z)}{\phi_2(z)}\right| - W_2(z)\right] - \frac{2z+k}{C_0} \\ & + \frac{1}{2}(k+2z)(2+3kz)C_0^{-3/2}\ln\left|\frac{\phi_3(z)}{\phi_4(z)}\right|,\end{aligned} \tag{70}$$

where

$$\phi_1(z) = 2k^2z^2 - kz(2z+k)(z-a) + 2k|z|\sqrt{R(z,-a)}, \tag{71}$$

$$\phi_2(z) = 2k^2z^2 - kz(2z+k)(b+z) + 2k|z|\sqrt{R(z,b)}, \tag{72}$$

$$\phi_3(z) = 2\sqrt{C_0 R(z,b)} + 2(b+z)C_0 - kz(2z+k), \tag{73}$$

and

$$\phi_4(z) = 2\sqrt{C_0 R(z,-a)} + 2(z-a)C_0 - kz(2z+k). \tag{74}$$

It is not difficult to verify that $\phi_3(z) = \psi_3(z)$ and $\phi_4(z) = \psi_4(z)$. Therefore, according to Eq. (37),

$$\frac{\phi_3(z)}{\phi_4(z)} = \left(\frac{\sqrt{C_0}+1}{\sqrt{C_0}-1}\right)^2. \tag{75}$$

On the other hand, it is shown in Appendix A that

$$\frac{\phi_1(z)}{\phi_2(z)} = \theta(-z)\left(\frac{z-a}{z+b}\right)^2. \tag{76}$$

We next substitute Eqs. (75) and (76) into Eq. (70), and then the resultant equation further into Eq. (67). The result for Φ_3 is in this way obtained as

$$\Phi_3 = \int_{-a}^{b} dz \quad \ln|z| \Big[-\frac{2z+k}{C_0} - \frac{(a-z)(b+z)}{kz} W_2(z) + (2z+k)(2+3kz) C_0^{-3/2} Y(z) \Big]. \qquad (77)$$

By now we have virtually completed our task of reducing J_{23} in terms of one quadrature. By substituting Eqs. (56), (62), (64), and (77) into Eq. (52), we reorganize our result for J_{23} in the following form:

$$J_{23} = 8[P_0 + (k^2-1)P_1 + 2P_2 - kP_3], \qquad (78)$$

where

$$\begin{aligned} P_0 = & \quad 8k^2/3 \ln|k/2| - 4/3 \\ & + \ [2\ln 2 - 1 + \ln|ab|] ab \ln^2|b/a| \\ & + \ 2[k\ln 2 - b(4k^2 - 2k + 1)/3k] \ln b \\ & - \ 2[k\ln 2 - a(4k^2 + 2k + 1)/3k] \ln|a|, \end{aligned} \qquad (79)$$

$$P_1 = \int_{-a}^{b} dz \frac{1}{C_0} \ln|z|, \qquad (80)$$

$$P_2 = \int_{-a}^{b} dz \frac{1}{z} [\lambda W_1(z) - (b+z)(z-a) W_2(z)] \ln|z|, \qquad (81)$$

and

$$P_3 = \int_{-a}^{b} dz (k+2z)(2+3kz) C_0^{-3/2} Y(z) \ln|z|. \qquad (82)$$

It turns out that the integral in the expression for P_3 can be further refined. Indeed, it is shown in Appendix B that

$$\begin{aligned} P_3 = & \quad \frac{10}{3}(2k\ln|k/2| - 1/k) + 4(b\ln^2 b - a\ln^2|a|) \\ & + \ \frac{4}{3}(3\ln|2/k| - 5 + 1/k^2)(b\ln b - a\ln|a|) \\ & + \ \frac{1}{3k}(b\ln b + a\ln|a|) + \frac{1}{k}(k^2-1)P_1. \end{aligned} \qquad (83)$$

Remarkably, it can be seen from Eq. (83) that the combination form of $(k^2-1)P_1 - kP_3$, the form in which P_1 and P_3 enter the right hand side of Eq. (78), can be fully reduced to an explicit form with no more integral in it. In this light we substitute Eqs. (79) and (83) into Eq. (78) to obtain the final expression for J_{23} as the following:

$$J_{23} = 8[g(k) + 2P_2], \qquad (84)$$

where

$$\begin{aligned} g(k) = \ & 2 + 4k^2\ln|2/k| + ab\ln|ab|\ln^2|b/a| + ab(2\ln 2 - 1)\ln^2|b/a| + 4k(a\ln^2|a| - b\ln^2 b) \\ & + [2k^2 + 9k/2 - 2/k - 2k(k+1)\ln 2 + 4kb\ln k] \ln b \\ & + [2k^2 - 9k/2 + 2/k + 2k(1-k)\ln 2 - 4ka\ln k] \ln|a|. \end{aligned} \qquad (85)$$

V. I(K) EXPRESSED IN TERMS OF ONE QUADRATURE; AND FURTHER IN TERMS OF SERIES

Further substitution of Eq. (42) and Eq. (84) into Eq. (18) then leads to

$$I(k) = -\frac{1}{2k^2}[g_0(k) + 2P_2], \qquad (86)$$

where

$$\begin{aligned} g_0(k) = & \quad 2k(a\ln^2|a| - b\ln^2 b) + ab\ln|ab|\ln^2|b/a| \\ & - \ 2(b\ln b - a\ln|a| - k - k\ln|k/2|)^2 \\ & + \ 2k^2(1 + \ln^2|k/2|). \end{aligned} \qquad (87)$$

As a consequence, we have accomplished reducing $I(k)$ in terms of one quadrature. Equation (86) will be further refined in the next section into the following final form:

$$\begin{aligned} I(k) \ = \ & \frac{1}{2k^2}\Bigg[b\ln^2\left|\frac{b}{a}\right| \left(\frac{1}{3}a\ln\left|\frac{b}{a}\right| + b\right) \\ & + \int_{a^2}^{b^2} dx \frac{1}{x-a^2} \ln\left|\frac{x}{a^2}\right| \left(\frac{1}{2}ab\ln\left|\frac{x}{b^2}\right| - k\right)\Bigg], \end{aligned} \qquad (88)$$

or,

$$\begin{aligned} I(k) \ = \ & \frac{1}{2k^2}\Bigg[a\ln^2\left|\frac{a}{b}\right| \left(\frac{1}{3}b\ln\left|\frac{a}{b}\right| + a\right) \\ & + \int_{1}^{a^2/b^2} dx \frac{1}{1-x} \left(\frac{1}{2}ab\ln\left|\frac{a^2}{b^2 x}\right| - k\right) \ln x \Bigg]. \end{aligned} \qquad (89)$$

The resulting expression for $I(k)$ is amazingly simple, in constract to its original six-fold integral form. Equation

(3) in the Introduction is obtained from Eq. (88) together with Eq. (6).

The one quadrature in Eq. (88) presents no numerical difficulty in applications. This is particularly so with the aid of the expansion forms in the limiting cases obtained in Sec. VII below. But it turns out that we have even a better choice. In this section, a series representation for $I(k)$ is developed. To this end, we rewrite Eq. (89) as

$$I(k)=\frac{1}{2k^2}\left[a\ln^2\left|\frac{a}{b}\right|\left(\frac{1}{3}b\ln\left|\frac{a}{b}\right|+a\right)+\left(ab\ln\left|\frac{a}{b}\right|-k\right)\frac{\pi^2}{6}+ab\zeta(3)+\int_0^{a^2/b^2}dx\frac{1}{1-x}\left(\frac{1}{2}ab\ln\left|\frac{a^2}{b^2x}\right|-k\right)\ln x\right]. \tag{90}$$

In obtaining Eq. (90) we have employed identities

$$\int_0^1 dx\frac{1}{1-x}\ln x=-\frac{\pi^2}{6}, \tag{91}$$

and

$$\int_0^1 dx\frac{1}{1-x}\ln^2 x=2\zeta(3). \tag{92}$$

We now employ series representation $1/(1-x)=\sum_{l=0}^{\infty}x^l$ in Eq. (90) to obtain

$$I(k)=\frac{1}{2k^2}\left[f_0(k)+\sum_{n=1}^{\infty}f_n(k)\right], \tag{93}$$

where

$$\begin{aligned} f_0(k) &= a\ln^2\left|\frac{a}{b}\right|\left(\frac{1}{3}b\ln\left|\frac{a}{b}\right|+a\right)-\frac{\pi^2}{6}k+ab\zeta(3)-\frac{a^3}{2b}\\ &+ \left(\frac{\pi^2}{6}ab+2k\ln\left|\frac{2k}{b^2}\right|\right)\ln\left|\frac{a}{b}\right|\\ &+ \left(\frac{a}{b}\right)^2\left[1+\left(\frac{a}{2b}\right)^2\right]\left[k-ab\left(\frac{1}{2}+\ln\left|\frac{b}{a}\right|\right)\right], \end{aligned} \tag{94}$$

and

$$f_n(k)=\left(ab\ln\left|\frac{a}{b}\right|+k-\frac{ab}{n+2}\right)\frac{1}{(n+2)^2}\left(\frac{a}{b}\right)^{2(n+2)}. \tag{95}$$

We emphasize that the series on the right hand side of Eq. (93) converge for all $k\geq 0$ and in effect the value of $I(k=0)=-1$ can be equally (and rather easily indeed) obtained from Eq. (93) by employing the following identity,

$$\sum_{n=1}^{\infty}\frac{1}{n^p}=\zeta(p), \tag{96}$$

with $\zeta(2)=\pi^2/6$ explicitly. The series representation of Eq. (93) for $I(k)$ should be particularly useful for analytical purposes.

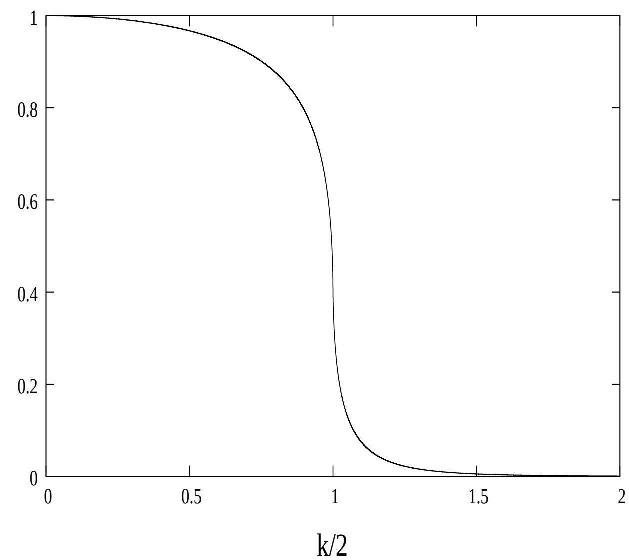

FIG. 1: The result for the quantity $-I(k)$, calculated with both of Eq. (86) of this paper and Eq. (29) of Ref. [23].

VI. DERIVATION OF EQ. (88) AND PROOF OF THE EQUIVALENCE OF IT AND THE CORRESPONDING ONE OF EQ. (29) IN REF. [23]

It is by no means evident that $I(k)$ given as Eq. (86) is equal to the corresponding one of Eq. (29) in Ref. [23]. In fact the present author had certain reservations about Eq. (29) of Ref. [23] for the mathematical assumption used in deriving it, and was convinced of its correctness only after a numerical check with Eq. (86). The numerical results from both of the expressions (before the rigorous proof of their equivalence was found) are shown in Fig. 1. They attain the same illustration. Besides, it can be derived analytically from Eq. (86) that $I(k=2)=-\pi^2/24$ [see also Eq. (143) and Eq. (144) below], which is the same as that derived from Eq. (29) of Ref. [23]. In this section we prove their equivalence by refining both of them into the form of Eq. (88).

We first refine the quantity given in Eq. (29) of Ref. [23] into the form of Eq. (88). For the purpose of convenience, we call it $I^{EV}(Q)$ (with $Q=k/2$). To this end,

we make the use of the following identity,

$$\int_0^Q dx\frac{1-x^2}{x^2} \quad \ln^3\left|\frac{1+x}{1-x}\right| = -(Q+\frac{1}{Q})\ln^3\left|\frac{1+Q}{1-Q}\right| +6\int_0^Q dx\frac{1+x^2}{x(1-x^2)}\ln^2\left|\frac{1+x}{1-x}\right|, \quad (97)$$

to rewrite Eq. (29) of Ref. [23] as

$$I^{EV}(Q) = \omega_1 \; + \; \omega_2\int_0^Q dx\frac{1+x^2}{x(1-x^2)}\ln^2\left|\frac{1+x}{1-x}\right| + \; \omega_3\int_0^Q dx\frac{1-x^2}{x^2}\ln^2\left|\frac{1+x}{1-x}\right|, \quad (98)$$

where

$$\omega_1 = -\frac{1-Q^4}{16Q^3}\ln^3\left|\frac{1+Q}{1-Q}\right|, \quad \omega_2 = \frac{1-Q^2}{4Q^2}, \quad (99)$$

$$\omega_3 = -\frac{1}{8}\left(\frac{1}{Q}+\frac{1-Q^2}{2Q^2}\ln\left|\frac{1+Q}{1-Q}\right|\right). \quad (100)$$

We next make the variable transform $x=(y-a)/(y+a)$ in Eq. (98) to obtain

$$I^{EV}(Q) = \omega_1 + \int_a^b dy \; \left[\; \omega_2(y^4-a^4) + 8\omega_3 a^2 y^2 \; \right] \frac{1}{y(y^2-a^2)^2}\ln^2\left|\frac{y}{a}\right|. \quad (101)$$

Further algebra then leads to

$$I^{EV}(Q) \;=\; \omega_1 - \left[\frac{\omega_2}{3}\ln\left|\frac{b}{a}\right| + \frac{2a^2\omega_3}{k}\right]\ln^2\left|\frac{b}{a}\right| + \int_{a^2}^{b^2} dy\left[\frac{\omega_2}{4}\ln\left|\frac{y}{a^2}\right| + \frac{2\omega_3 a^2}{y}\right]\frac{1}{y-a^2}\ln\left|\frac{y}{a^2}\right|. \quad (102)$$

The remaining derivation to obtain the form of Eq. (88) is routine.

We next refine $I(k)$ of Eq. (86) into Eq. (88). To this end, we carry out partial integration on the right hand side of Eq. (81) to rewrite it as

$$P_2 = k[b\ln^2 b\ln|2b/k| - a\ln^2|a|\ln|2a/k|] + \bar{P}_2, \quad (103)$$

with

$$\bar{P}_2 = \frac{1}{2}\int_{-a}^{b} dz[(2z-k)W_1(z) + (2z+k)W_2(z)]\ln^2|z|. \quad (104)$$

With some straightforward algebra, $\bar{P}_2$ can be put into the form

$$\bar{P}_2 = (t_1 - 4kt_2 - 4kt_3 - t_4)/8, \quad (105)$$

where

$$t_1 = \int_{a^2}^{b^2} dy\ln^2 y\ln|y-a^2|, \quad (106)$$

$$t_2 = \int_{|a|}^{b} dy\ln^2 y\ln\left|\frac{y+a}{y-a}\right|, \quad (107)$$

$$t_3 = \int_{|a|}^{b} dy\ln^2 y\ln\left|\frac{y+b}{y-b}\right|, \quad (108)$$

and

$$t_4 = \int_{a^2}^{b^2} dy\ln^2 y\ln|y-b^2|. \quad (109)$$

The next manipulation is the key to the procedure. For t_1 we perform further partial integration to obtain

$$t_1 \;=\; [b^2(d_4^2+1) - a^2(d_1^2+1)]\ln|2k| - \int_{a^2}^{b^2} dy\frac{1}{y-a^2}[y(\ln^2 y - 2\ln y + 2) - a^2(d_1^2+1)], \quad (110)$$

where

$$d_1 \;=\; 2\ln|a| - 1, \quad d_2 = 2(\ln|a|-1),$$
$$d_3 \;=\; 2(1-\ln b), \quad d_4 = -2\ln b + 1, \quad (111)$$

with d_2, d_3 for later quotations. Further algebra then yields

$$t_1 = b^2(d_4^2+1)\ln|2k| - (d_1^2+1)(2k + a^2\ln|2k|) - \Xi_1, \quad (112)$$

where

$$\Xi_n = \int_{a^2}^{b^2} dy\frac{y^{2-n}}{y-a^2}\left(2d_n + \ln\left|\frac{y}{a^2}\right|\right)\ln\left|\frac{y}{a^2}\right|, \quad (113)$$

with Ξ_2, Ξ_3, and Ξ_4 for later quotations. Similarly we can obtain

$$t_2 = \frac{1}{4}[b(d_3^2+4)\ln|2/k| - a(d_2^2+4)\ln|2a^2/k| + a\Xi_2]. \quad (114)$$

For t_4 we first perform partial integration to get

$$t_4 \;=\; [b^2(d_4^2+1) - a^2(d_1^2+1)]\ln|2k| - \int_{a^2}^{b^2} dx\frac{1}{x-b^2}[x(\ln^2 x - 2\ln x + 2) - b^2(d_4^2+1)]. \quad (115)$$

We then make further variable tranform $x = a^2b^2/y$ to get

$$t_4 = (d_4^2+1)(b^2\ln|2k| - 2k) - a^2(d_1^2+1)\ln|2k| + a^4b^2\Xi_4. \quad (116)$$

Similarly we can obtain

$$t_3 = \frac{1}{4}[a(d_2^2+4)\ln|k/2| + b(d_3^2+4)\ln|2b^2/k| - a^2 b\Xi_3]. \tag{117}$$

Substitution of Eqs. (112), (114), (116), (117) into Eq. (103) yields

$$\begin{aligned} P_2 = &\quad k(\ln b - 1)(\ln b + 2b\ln|2b/k|) \\ &- \ k(\ln|a| - 1)(\ln|a| + 2a\ln|2a/k|) - T/2, \end{aligned} \tag{118}$$

where

$$T = [\Xi_1 + ka\Xi_2 - kba^2\Xi_3 + a^4 b^2 \Xi_4]/4, \tag{119}$$

which has the following explicit expression:

$$T = [2k\ln|ab| + b(b-2a+2a\ln b)\ln|b/a| - 2k - 2ab/3\ln^2|b/a|]\ln|b/a| + \int_{a^2}^{b^2} dx \frac{1}{x-a^2}\ln\left|\frac{x}{a^2}\right|\left(\frac{1}{2}ab\ln\left|\frac{x}{b^2}\right| - k\right). \tag{120}$$

One then substitutes Eq. (118) together with Eq. (120) into Eq. (86) for $I(k)$. The remaining derivation to get the form of Eq. (88) becomes routine.

VII. EXPANSIONS IN THE LIMITING CASES

The limiting structures of $\Pi_1(k,0)$ at $k=0$, $k=2$, and at large k have various physical implications and deserve particular attention. In virtue of our proof of the correctness of the main conclusion of Engel and Vosko's theory in Ref. [23], there is no doubt that the expansions obtained by them in the limiting cases [i.e., Eqs. (30), (31), and (32) in Ref. [23]] must also be right. Indeed they are all confirmed with calculations based on Eq. (89). We sketch the calculations below.

It turns out that the expression (89) is rather suitable for deriving the expansions. We first consider the cases of $k \to 0$ and $k \to \infty$, To this end, we make the variable transform $x = [(1-y)/(1+y)]^2$ in Eq. (89) and bring it into another form,

$$I(k) = \frac{1}{2k^2}\left[b\ln^2\left|\frac{b}{a}\right|\left(\frac{1}{3}a\ln\left|\frac{b}{a}\right| + b\right) + 2\int_0^Q dy\left(\frac{1}{y} + \frac{2}{1-y}\right)\ln\left|\frac{1+y}{1-y}\right|\left(ab\ln\left|\frac{a(1+y)}{b(1-y)}\right| - k\right)\right]. \tag{121}$$

We act the operator of $\frac{1}{2}(1-Q^2)\frac{\partial}{Q\partial Q} + 1$ on the quantity $I(k)Q^2$. With some algebra, one can obtain

$$\left[\frac{1}{2}(1-Q^2)\frac{\partial}{Q\partial Q} + 1\right][I(k)Q^2] = \frac{1}{4Q}\left[b\ln^2\left|\frac{b}{a}\right| - 2\int_0^Q dy\left(\frac{1}{y} + \frac{2}{1-y}\right)\ln\left|\frac{1+y}{1-y}\right|\right]. \tag{122}$$

One then acts further the operator of $(1/Q)\partial/\partial Q$ (which is of course just $2\partial/\partial Q^2$) on the both sides of the preceding expression. This action yields the following result,

$$\frac{\partial}{Q\partial Q}\left[\frac{1}{2}(1-Q^2)\frac{\partial}{Q\partial Q} + 1\right][I(k)Q^2] = \frac{1}{4Q^3}F(Q), \tag{123}$$

where

$$\begin{aligned} F(Q) = &\ -\ \ln\left|\frac{b}{a}\right|\left(\ln\left|\frac{b}{a}\right| + 2\right) \\ &+\ 2\int_0^Q dy\left(\frac{1}{y} + \frac{2}{1-y}\right)\ln\left|\frac{1+y}{1-y}\right|. \end{aligned} \tag{124}$$

It can be readily shown that

$$F(Q \to 0) = 4\sum_{n=0}^{\infty}\frac{1}{2n+3}\left[2\Psi(n) + \frac{1}{2n+3} - 1\right]Q^{2n+3}, \tag{125}$$

and

$$F(Q \to \infty) = 4\sum_{n=0}^{\infty}\frac{1}{2n+3}\left[2\Psi(n) + \frac{1}{2n+3} - 1\right]\frac{1}{Q^{2n+3}}, \tag{126}$$

where

$$\Psi(n) = \sum_{l=0}^{n}\frac{1}{2l+1}. \tag{127}$$

In passing we note the remarkable symmetry in the above two forms. For $k \to 0$ we have, from Eq. (123) and Eq. (125),

$$\frac{\partial}{Q\partial Q}\left[\frac{1}{2}(1-Q^2)\frac{\partial}{Q\partial Q}+1\right][I(k)Q^2] = \sum_{n=0}^{\infty}\frac{1}{2n+3}\left[2\Psi(n)+\frac{1}{2n+3}-1\right]Q^{2n}. \quad (128)$$

With Eq. (128), it is straightforward to determine the expansion for $I(k \to 0)$. To this end, we write

$$I(k \to 0) = -1 + \sum_{n=1}^{\infty} c_n Q^{2n}, \quad (129)$$

where c_n are the coefficients we have to determine. To write the preceding form, we have made the use of the truth of $I(k=0) = -1$ which can be readily obtained from Eq. (121) and is in fact well known [11, 21–23]. The fact that the expansion retains only even powers of Q is evident from Eq. (128). [In fact $I(k)$, which is defined physically only for $k \geq 0$, is an even function if extended to the range of $k < 0$. This fact can be best appreciated from Eq. (98), but also in another interesting way. Upon making the variable tranform $x = 1/y$ in Eq. (89), one can bring it into yet another form,

$$I(k) = \frac{1}{2k^2}\left[b\ln^2\left|\frac{b}{a}\right|\left(\frac{1}{3}a\ln\left|\frac{b}{a}\right|+b\right) + \int_1^{b^2/a^2}dx\frac{1}{x-1}\left(\frac{1}{2}ab\ln\left|\frac{a^2x}{b^2}\right|-k\right)\ln x\right]. \quad (130)$$

But, on the other hand, the right hand side of the above equation can be exactly obtained from that of Eq. (89) by merely changing k to $-k$. Thus $I(k) = I(-k)$.] We then substitute Eq. (129) into the left hand side of Eq. (128). By equating the coefficients of the same powers of Q^2 on both sides of the resulting equation, we obtain, for $n \geq 1$,

$$(n+1)(n+2)c_{n+1} - n(n+1)c_n = \frac{1}{2(2n+3)}\left[2\Psi(n)+\frac{1}{2n+3}-1\right], \quad (131)$$

or further

$$n(n+1)c_n = \frac{1}{2}\sum_{l=1}^{n}\frac{1}{2l+1}\left[2\Psi(l-1)+\frac{1}{2l+1}-1\right]. \quad (132)$$

By the use of Eq. (127), we have

$$n(n+1)c_n = \frac{1}{2}\sum_{l=1}^{n}[\Psi(l)-\Psi(l-1)][\Psi(l)+\Psi(l-1)-1]. \quad (133)$$

After carrying out the above summation we have, with the aid of the fact $\Psi(0) = 1$,

$$c_n = \frac{\Psi(n)[\Psi(n)-1]}{2n(n+1)}, \quad (134)$$

and accordingly

$$I(k \to 0) = -1 + \frac{1}{2}\sum_{n=1}^{\infty}\frac{\Psi(n)[\Psi(n)-1]}{n(n+1)}Q^{2n}. \quad (135)$$

Equation (135) is the same as Eq. (30) of Ref. [23].

In particular, the leading two terms in Eq. (135) which are

$$I(k \to 0) = -1 + \frac{1}{9}Q^2 + ..., \quad (136)$$

had been obtained numerically by Kleinman and Lee [21] and later by Chevary and Vosko [22] (who also obtained the next order $46Q^4/675$ correctly). The form in Eq. (136) yields the following leading gradient correction [15, 28–32] to the local density approximation of Kohn-Sham exchange energy density [21–23]

$$\triangle E_x^{(1)} = -\frac{5e^2}{216\pi(3\pi^2)^{1/3}}\int d\mathbf{r}\frac{[\nabla n(\mathbf{r})]^2}{[n(\mathbf{r})]^{4/3}}. \quad (137)$$

The leading gradient correction to the Kohn-Sham exchange energy was investigated originally by Sham [33], but he got the coefficient to be $-7e^2/[432\pi(3\pi^2)^{1/3}]$ instead by employing screened Coulomb potential with screening going to zero (see also Ref. [34]). Later Gross and Dreizler [35] (see also Ref. [36]) got the same result as Sham's, essentially employing also screened Coulomb potential (with screening going to zero). This well-known controversy has been one of the major causes inspiring the investigations of the exact structures of $\Pi_1(\mathbf{k}, 0)$, and has been effectively elucidated in Refs. [21–23]. Our result based on the rigorous derivation helps to *give a final settlement of the controversy itself*. Questions such as whether $\triangle E_x^{(1)}$ in Eq. (137) or the one by Sham should be added to the type of Ma-Brueckner's gradient correction to the correlation energy (to get the Kohn-Sham exchange-correlation energy beyond the local density approximation) remain open [21, 31].

For $k \to \infty$, we have, from Eq. (123) and Eq. (126),

$$\frac{\partial}{Q\partial Q}\left[\frac{1}{2}(1-Q^2)\frac{\partial}{Q\partial Q}+1\right][I(k)Q^2] = \sum_{n=0}^{\infty}\frac{1}{2n+3}\left[2\Psi(n)+\frac{1}{2n+3}-1\right]\frac{1}{Q^{2n+6}}. \quad (138)$$

It is not difficult to see from Eq. (138) that the expansion of $I(k)$ for large k commences with $O(1/Q^6)$, and accordingly it assumes the following general form,

$$I(k \to \infty) = \sum_{n=3}^{\infty}\tilde{c}_n\frac{1}{Q^{2n}}. \quad (139)$$

Substituting this form into Eq. (138), we obtain

$$(n+2)(n+3)\tilde{c}_{n+3} - (n+1)(n+2)\tilde{c}_{n+2} = \frac{1}{2(2n+3)}\left[1 - \frac{1}{2n+3} - 2\Psi(n)\right], \tag{140}$$

for $n \geq 1$. Similar procedure to that used above for the case of $k \to 0$ can be employed to obtain

$$\tilde{c}_n = -\frac{\Psi(n-2)[\Psi(n-2)-1]}{2(n-1)n}. \tag{141}$$

Thus

$$I(k \to \infty) = -\frac{1}{2}\sum_{n=1}^{\infty}\frac{\Psi(n)[\Psi(n)-1]}{(n+1)(n+2)}\frac{1}{Q^{2(n+2)}}, \tag{142}$$

confirming Eq. (31) in Ref. [23], (there is a sign error in the first identity of that equation.) We note that the leading two terms of Eq. (142) had been reported by Geldart and Taylor [12] (see also Ref. [14]); the leading term had also been obtained by Kleinman [26, 34].

We next give the expansion near $k = 2$. With the aid of Identity (91), the characteristic property of $I(k = 2) = -\pi^2/24$ and the leading singular term (meaning the most divergent term upon derivative with respect to k) can be immediately seen from Eq. (89) to be:

$$I(k \to 2) = -\frac{\pi^2}{24} + \frac{1}{12}a\ln^3\left|\frac{a}{2}\right|. \tag{143}$$

The conclusion drawn in Ref. [23] that the singularity of $\Pi_1(\mathbf{k}, 0)$ dominates that of $\Pi_0(\mathbf{k}, 0)$ is corroborated. In general, we obtain

$$\begin{aligned} I(k \to 2) = \frac{1}{8}\Bigg\{ & -\frac{\pi^2}{3} + \left(2\zeta(3) - \frac{\pi^2}{3}\right)a + \left(3\zeta(3) - \frac{\pi^2}{6} + \frac{1}{2}\right)a^2 + \left(4\zeta(3) - \frac{\pi^2}{24}\right)a^3 + \left(5\zeta(3) + \frac{11\pi^2}{144} - \frac{37}{96}\right)a^4 \\ & + \left(6\zeta(3) + \frac{37\pi^2}{192} - \frac{125}{192}\right)a^5 + \ldots \\ & + \frac{1}{3}\sum_{n=1}^{\infty}(n+1)a^n\ln^3\left|\frac{a}{2}\right| + a^2\sum_{n=0}^{\infty}e_n a^n\ln^2\left|\frac{a}{2}\right| + a\left[\frac{\pi^2}{3} + \left(\frac{\pi^2}{2} - 1\right)a + \sum_{n=2}^{\infty}r_{n+1}a^n\right]\ln\left|\frac{a}{2}\right|\Bigg\}, \end{aligned} \tag{144}$$

where

$$e_n = 2(n+1) + \sum_{l=0}^{n}\frac{l-n}{(l+1)(l+2)}\frac{1}{2^{l+1}}, \tag{145}$$

and

$$r_n = \frac{\pi^2}{6}(n+1) + 7(n-1) - 8\phi(n-2) + \sum_{m=3}^{n}\frac{(n-m+1)}{(m-1)(m-2)}2^{3-m}\left[-1 + \phi(m-1) + \frac{3(m-1)^2-1}{m(m-1)(m-2)} - \sum_{l=1}^{m}\frac{1}{l}2^l\right], \tag{146}$$

with $\phi(m) = \sum_{l=0}^{m} 1/(l+1)$. In particular, $e_0 = 2$, $e_1 = 15/4$, $e_2 = 131/24$, and $e_3 = 229/32$; $r_3 = 2\pi^2/3$, $r_4 = 5\pi^2/6 + 13/8$, and $r_5 = \pi^2 + 173/48$. Equation (144) confirms Eq. (32) in Ref. [23] in virtue of the following identities,

$$\begin{aligned} &\int_0^1 dx\frac{1-x^2}{x^2}\ln^3\left|\frac{1+x}{1-x}\right| \\ &= 6\left[\int_0^1 dy\frac{1}{1-y}\ln^2 y - \int_0^1 dy\frac{1}{1+y}\ln^2 y\right] \\ &= 3\zeta(3), \end{aligned} \tag{147}$$

where $\zeta(3) = 1.202056903\ldots$. We would like to point out in this connection that Eq. (21) in Ref. [24] is at variance with Eq. (32) in Ref. [23] and accordingly also with Eq. (144) above.

Appendix A: Verification for Eqs. (36), (37), and (76)

It is worth pointing out first the following fact,

$$(1+k)z + b \geq 0, \quad \textit{and} \quad (k-1)z + a \geq 0, \tag{A1}$$

which can be readily verified for $-a \leq z \leq b$. Accordingly,

$$\sqrt{R(z,b)} = (1+k)z + b; \quad \sqrt{R(z,-a)} = (k-1)z + a. \tag{A2}$$

A direct substitution of Eq. (24) and Eq. (A2) into Eq. (31) and Eq. (32), respectively, leads to

$$\psi_1(z) = 4b^2 z(z+a), \quad and \quad \psi_2(z) = k^2 z(z+a), \quad \text{(A3)}$$

for $z > 0$; and

$$\psi_1(z) = k^2 z(z-b), \quad and \quad \psi_2(z) = 4a^2 z(z-b), \quad \text{(A4)}$$

for $z < 0$. Equation (36) is hence verified. Equation (76) can be verified in the same manner.

We next verify Eq. (37). Once again we make a direct substitution of Eq. (24) and Eq. (A2) into Eq. (33) and Eq. (34), respectively. By carrying out some algebra, we can obtain

$$\psi_3(z) = \frac{1}{2k} \quad [\quad C_0^2 + 2(k+1)C_0^{3/2} + k(k+4)C_0 + \ 2(k^2+k-1)\sqrt{C_0} + k^2 - 1], \quad \text{(A5)}$$

and

$$\psi_4(z) = \frac{1}{2k} \quad [\quad C_0^2 + 2(k-1)C_0^{3/2} + k(k-4)C_0 + \ 2(-k^2+k+1)\sqrt{C_0} + k^2 - 1]. \quad \text{(A6)}$$

Both of these forms can be factorized, and the result is

$$\psi_3(z) = \frac{1}{2k}(\sqrt{C_0}+1)^2(\sqrt{C_0}+k+1)(\sqrt{C_0}+k-1), \quad \text{(A7)}$$

and

$$\psi_4(z) = \frac{1}{2k}(\sqrt{C_0}-1)^2(\sqrt{C_0}+k+1)(\sqrt{C_0}+k-1). \quad \text{(A8)}$$

Equation (37) is as a consequence established.

Appendix B: Evaluation for η_n in Eq. (41) and derivation for Eq. (83)

An efficient way to evaluate η_n and P_3 is to introduce the variable transform, $z = \frac{1}{2k}(y^2-1)$, which casts Eq. (41) in the form

$$\eta_n = \int_{|1-k|-1}^{k} dy (y+1)^{n+1} \ln\left|\frac{y+2}{y}\right|. \quad \text{(B1)}$$

The remaining calculation for η_n is then routine. The explicit expressions for η_1, η_{-1}, and η_{-3} are given as follows,

$$\eta_1 = \frac{2}{3}[2k + (k^2+k+1)b\ln|2b| - (k^2-k+1)a\ln|2a| - k(k^2+3)\ln k], \quad \text{(B2)}$$

$$\eta_{-1} = 2(b\ln|2b| - a\ln|2a| - k\ln k), \quad \text{(B3)}$$

and

$$\eta_{-3} = 2\left[\frac{k}{k^2-1}\ln k + \ln\left|\frac{k+1}{k-1}\right| - \frac{b}{k+1}\ln|2b| + \frac{a}{1-k}\ln|2a|\right]. \quad \text{(B4)}$$

We next evaluate P_3 to verify Eq. (83). With the transform $z = \frac{1}{2k}(y^2-1)$, Eq. (82) can be rewritten as

$$P_3 = \frac{1}{2k^2}\sum_{n=-1}^{1}\gamma_n \int_{|1-k|}^{1+k} dy y^{2n} \ln\left|\frac{y^2-1}{2k}\right| \ln\left|\frac{y+1}{y-1}\right|, \quad \text{(B5)}$$

where

$$\gamma_1 = 3, \quad \gamma_0 = 3k^2 - 2, \quad \gamma_{-1} = k^2 - 1. \quad \text{(B6)}$$

One then carries out partial integration to bring Eq. (B5) into the following form,

$$P_3 = \frac{1}{2k^2}\sum_{n=-1}^{1}\gamma_n \frac{1}{2n+1}\left[(1+k)^{2n+1}\ln b \ln\left|\frac{2b}{k}\right| - \tilde{k}^{2n+1}\ln|a|\ln\left|\frac{\tilde{k}+1}{\tilde{k}-1}\right| + \Omega_n\right], \quad \text{(B7)}$$

with $\tilde{k} = |1-k|$ and Ω_n defined as

$$\Omega_n = \int_{\tilde{k}}^{1+k} dy y^{2n+1}\left[\frac{1}{y+1}\ln\left|\frac{2k}{(y+1)^2}\right| - \frac{1}{y-1}\ln\left|\frac{2k}{(y-1)^2}\right|\right], \quad \text{(B8)}$$

for $n = 1, 0, -1$. The Ω_{-1} can be evaluated as

$$\Omega_{-1} = h_0(k) - 2k \int_{-a}^{b} dz \frac{1}{C_0} \ln |z|, \tag{B9}$$

where

$$h_0(k) = \ln |2k| \ln \left|\frac{a}{b}\right| + \ln^2 |2b| - \ln^2 |\tilde{k}+1| + \ln^2 k - \ln^2 |\tilde{k}-1|. \tag{B10}$$

For $n = 0, 1$, one has

$$\Omega_n = \int_{\tilde{k}+1}^{2b} dx (x-1)^{2n+1} \frac{1}{x} \ln\left|\frac{2k}{x^2}\right| - \int_{\tilde{k}-1}^{k} dx (x+1)^{2n+1} \frac{1}{x} \ln\left|\frac{2k}{x^2}\right|, \tag{B11}$$

or

$$\Omega_n = \sum_{m=1}^{2n+1} C_{2n+1}^m \left[(-)^m \int_{\tilde{k}+1}^{2b} dx x^{m-1} \ln\left|\frac{2k}{x^2}\right| - \int_{\tilde{k}-1}^{k} dx x^{m-1} \ln\left|\frac{2k}{x^2}\right| \right]. \tag{B12}$$

By carrying out the integrals on the right hand side of Eq. (B12), we obtain, for $n = 0, 1$,

$$\begin{aligned} \Omega_n = h_0(k) + \sum_{m=1}^{2n+1} C_{2n+1}^m \frac{1}{m^2} (-)^m \Bigg[(2b)^m \left(m \ln\left|\frac{2b^2}{k}\right| - 2 \right) + (-k)^m \left(m \ln\left|\frac{k}{2}\right| - 2 \right) \\ + (\tilde{k}+1)^m \left(m \ln\left|\frac{2k}{(\tilde{k}+1)^2}\right| + 2 \right) + (1-\tilde{k})^m \left(m \ln\left|\frac{2k}{(\tilde{k}-1)^2}\right| + 2 \right) \Bigg]. \end{aligned} \tag{B13}$$

One then substitutes Eqs. (B9) and (B13) into Eq. (B7) to obtain, with some further algebra, Eq. (83). Or one can obtain first explicit expressions for Ω_0 and Ω_1. In that case, one has

$$\Omega_0 = h_0(k) + 2[k \ln k - 2b \ln |2b| + (\tilde{k}+1) \ln |\tilde{k}+1| - (\tilde{k}-1) \ln |\delta - 1|], \tag{B14}$$

and

$$\begin{aligned} \Omega_1 = h_0(k) + \frac{1}{3} \quad [\quad & -20k - 12k \ln 2 + k(6 + 9k + 2k^2) \ln k - 2b(8 - k + 2k^2) \ln |2b| + (\tilde{k}+1)(11 - 5\tilde{k} + 2\tilde{k}^2) \ln |\tilde{k}+1| \\ - \quad & (\tilde{k}-1)(11 + 5\tilde{k} + 2\tilde{k}^2) \ln |\tilde{k}-1|]. \end{aligned} \tag{B15}$$

In any case, the remaining derivation to obtain Eq. (83) is straightforward.

[1] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems*, (Dover, New York, 2003).
[2] D. Pines and P. Nozières, *The Theory of Quantum Liquids*, (Perseus Books, Massachusetts, 1999).
[3] C. A. Burns, P. Giura, A. Said, A. Shukla, G. Vankó, M. Tuel-Benckendorf, E. D. Isaacs, and P. M. Platzman, Phys. Rev. Lett. **89**, 236404 (2002).
[4] S. Waidmann, M. Knupfer, B. Arnold, J. Fink, A. Fleszar, and W. Hanke, Phys. Rev. B **61**, 10149 (2000).
[5] W. Schülke, J. Phys.: Condens. Matter **13**, 7557 (2001).
[6] S. Huotari, M. Cazzaniga, H.-Ch. Weissker, T. Pylkkänen, H. Müller, L. Reining, G. Onida, and G. Monaco, Phys. Rev. B **84**, 075108 (2011).
[7] S. H. Glenzer and R. Redmer, Rev. Mod. Phys. **81**, 1625 (2009); the subject concerned in this review is of plasmas.
[8] J. Lindhard, K. Dan. Vidensk. Selskab, Mat-Fys. Medd. **28**, (8) (1954).
[9] D. Bohm and D. Pines, Phys. Rev. **92**, 609 (1953); M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957).
[10] J. Hubbard, Proc. Roy. Soc. **A243**, 336 (1957).
[11] D. F. DuBois, Ann. Phys. (N. Y.) **7**, 174 (1959).
[12] D. J. W. Geldart and R. Taylor, Can. J. Phys. **48**, 155 (1970); **48**, 167 (1970).
[13] F. Toigo and T. O. Woodruff, Phys. Rev. B **2**, 3958 (1970).
[14] D. J. W. Geldart, T. G. Richard, and M. Rasolt, Phys. Rev. B **5**, 2740 (1972).

[15] L. J. Sham, Phys. Rev. B **7**, 4357 (1973).

[16] D. N. Tripathy and S. S. Mandal, Phys. Rev. B **16**, 231 (1977).

[17] B. K. Rao, S. S. Mandal, and D. N. Tripathy, J. Phys. F **9**, L51 (1979).

[18] F. Brosens, L. F. Lemmens, and J. T. Devreese, Phys. Status Solidi B **74**, 45 (1976); F. Brosens, J. T. Devreese, and L. F. Lemmens, *ibid.* **80**, 99 (1977); J. T. Devreese, F. Brosens, and L. F. Lemmens, Phys. Rev. B **21**, 1349 (1980); F. Brosens, J. T. Devreese, and L. F. Lemmens, *ibid.* **21**, 1363 (1980).

[19] A. Holas, P. K. Aravind, and K. S. Singwi, Phys. Rev. B **20**, 4912 (1979); P. K. Aravind, A. Holas, and K. S. Singwi, *ibid.* **25**, 561 (1982).

[20] J. E. Alvarellos and F. Flores, J. Phys. F **14**, 1673 (1984).

[21] L. Kleinman and S. Lee, Phys. Rev. B **37**, 4634 (1988).

[22] J. A. Chevary and S. H. Vosko, Phys. Rev. B **42**, 5320 (1990).

[23] E. Engel and S. H. Vosko, Phys. Rev. B **42**, 4940 (1990).

[24] M. L. Glasser, Phys. Rev. B **51**, 7283 (1995).

[25] P. S. Svendsen and U. von Barth, Int. J. Quantum Chem. **56**, 351 (1995).

[26] P. R. Antoniewicz and L. Kleinman, Phys. Rev. B **31**, 6779 (1985).

[27] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series, and Products*, edited by A. Jeffrey and D. Zwillinger (Academic Press, 2000).

[28] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).

[29] S. K. Ma and K. A. Brueckner, Phys. Rev. **165**, 18 (1968).

[30] D. C. Langreth and J. P. Perdew, Phys. Rev. B **21**, 5469 (1980).

[31] D. C. Langreth and S. H. Vosko, Phys. Rev. Lett. **59**, 497 (1987), and references therein.

[32] R. M. Dreizler and E. K. U. Gross, *Density Functional Theory*, (Springer-Verlag, Berlin, 1990).

[33] L. J. Sham, in *Computational Methods in Band Theory*, edited by P. M. Marcus, J. F. Janak, and A. R. Williams (Plenum, New York, 1971), P. 458.

[34] L. Kleinman, in Phys. Rev. B **30**, 2223 (1984), also derived analytically (with bare Coulomb potential) a result of $I(k \to 0) = -1 + (2/9)Q^2$ (in the present terminology) which amounts to a coefficient of $-e^2/[54\pi(3\pi^2)^{1/3}]$ in $\triangle E_x^{(1)}$; this result was later disputed in Ref. [21]. On the other side, for large k he obtained in that paper $I(k \to 0) = -1/(27Q^6)$ which is confirmed here [see the remark below Eq. (142)].

[35] E. K. U. Gross and R. M. Dreizler, Z. Phs. A **302**, 103 (1981).

[36] A. -R. E. Mohammed and V. Sahni, Phys. Rev. B **29**, 3687 (1984).